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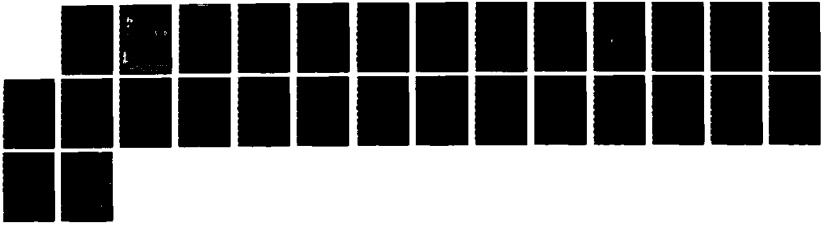

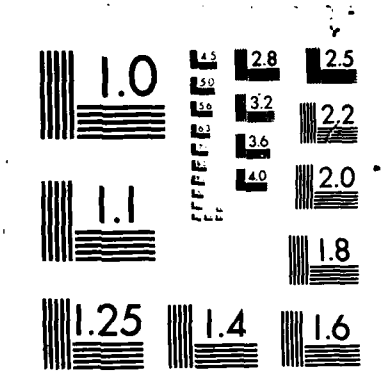

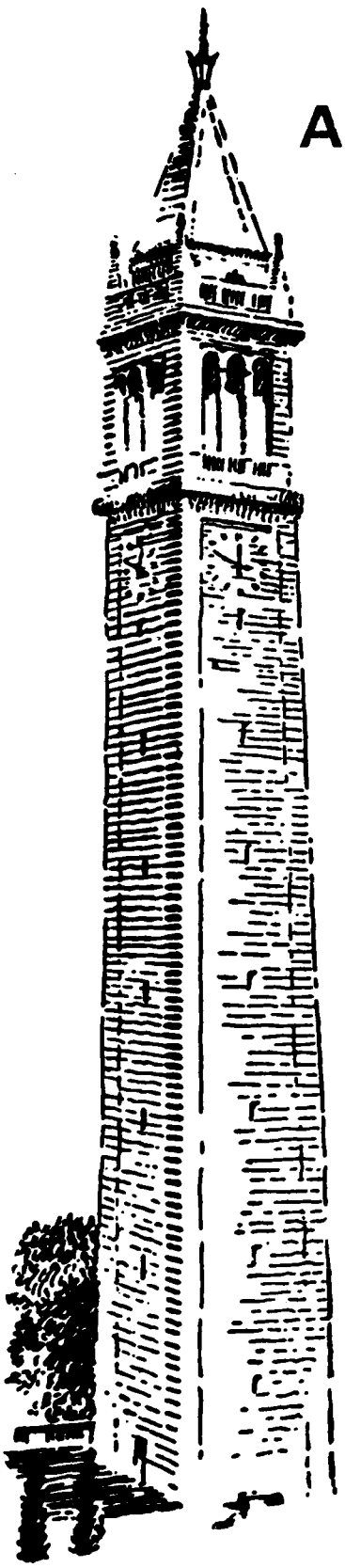

FIRST & SECOND QUARTER PROGRESS REPORT 1986 ON PLASMA THEORY AND SIMULATION

January 1 to June 30, 1986

DOE Contract DE-FG03-86ER53220
ONR Contract N00014-85-K-0809
Varian Gift and MICRO
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ELECTRONICS RESEARCH LABORATORY
College of Engineering
University of California, Berkeley, CA 94720

ANNOUNCEMENT

The Plasma Theory and Simulation Group in the EECS Department and ERL is pleased to announce receipt of three awards to its members.

The first is the appointment of Dr. Liu Chen as Visiting Miller Research Professor for an eight week visit during the 1987-88 academic year, to be hosted by our group in EECS, with Prof. Birdsall as faculty sponsor. Dr. Chen comes to us from Princeton University where he is Deputy Head of the theory group at the Princeton Plasma Physics Laboratory. Dr Chen received his Ph.D. while in our group in the early 1970's. It is expected that he will arrive in the Fall 1987 and interact with the plasma community which reaches across several department lines, as well as with researchers at LBL and LLNL.

The second is the award to Lou Ann Schwager of a U.S. Dept. of Energy Fusion Energy Postdoctoral Award, with appointment to be at the Sandia National Laboratories, Livermore. Ms. Schwager is now completing her dissertation on plasma-sheath-wall dynamics, including secondary electron emission and reflected ions, working in our PTSG, a student in NE. She will take up her post-doc about September 1. It is expected that she will split her time between Sandia, where Drs. Walter Bauer and Ken Wilson have excellent plasma-surface experimental facilities, and PTSG, where she will continue with her simulations. The award is one of three made nationally.

The third is the award to Richard Procassini of a DAAD (Deutscher Akademischer Austauschdienst) scholarship to continue his graduate plasma studies for a year at the University of Munich, Max Planck Institute for Plasma Physics, at Garching, working with our friend Dr. Roland Chodura. Mr. Procassini is an NE graduate student in PTSG, with much of his research supported by an IR&D grant from LLNL. He is working closely with Dr. Bruce Cohen at LLNL, on a large (full fusion machine particle simulation) code TESS, developed by Dr. Cohen and Prof. Birdsall. There is similar work at MPIPP, especially on the addition of Coulomb collisions.

The Plasma Theory and Simulation Group is now completing its 20th year, dating back to Prof. Birdsall's return from sabbatical in Japan with Prof. A. Hasegawa and T. Kamimura, and the appointment of Dr. A. B. Langdon to be our first post-doc. Fourteen Ph.D.s and six Masters have been granted in that period to students in the Group, and there have been six post-docs with two and three year terms. The major text in the area, *Plasma Physics via Computer Simulation (1985)*, by Birdsall and Langdon, has included much of the work of the Group, in methods and in applications. Students and post-docs have come from EECS, NE, Physics, Math and Astronomy and have moved on to work in a wide variety of engineering and scientific activities.

Looking forward to a second 20 years! Charles K. (Ned) Birdsall

20 April 1987 **With apologies for the gild on the lily!**

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Our group uses theory and simulation as tools in order to increase the understanding of plasma instabilities, heating, transport, plasma-wall interactions, and large potentials in plasmas. We also work on the improvement of simulation both theoretically and practically.

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Research in plasma theory and simulation, plasma-wall interactions, large potentials in plasmas.

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

See reverse side

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20. ABSTRACT

General Plasma Theory and Simulation

A. Computer simulation of bounded plasma systems, with external circuits, is discussed in considerable detail.

B. Artificial cooling of trapped electrons in bounded simulations was observed and is now attributed to noiseless injection; the cooling does not occur if random injection is used.

Plasma-Wall Physics, Theory and Simulation

A,B,C. The collector and source sheaths at the boundaries of warm plasma are treated in detail, including ion reflection and secondary electron emission at the collector.

*, ** D. The Kelvin-Helmholtz instability is observed in a self-consistent magnetized sheath, producing long-lived vortices which increase the particle transport to the wall dramatically.

Code Development and Software Distribution

A. The ES2 User's Manual--Version 1 has been issued.

B. Addition of electron-neutral elastic collisions is introduced.

*** C. Implicit particle simulation of velocity space transport and self-consistent electric potentials in magnetized plasmas (TESS Code) is described in detail.

D. Dynamic dimensioning with heap management is described in detail.

Major support is from DOE.

*Supported in part by ONR.

**Supported in part by Varian/MICRO.

***Supported in part by IR&D Grant from LLNL.

FIRST AND SECOND QUARTER PROGRESS REPORT
ON
PLASMA THEORY AND SIMULATION

January 1 to June 30, 1986

Our research group uses both theory and simulation as tools in order to increase the understanding of instabilities, heating, transport, plasma-wall interactions, and large potentials in plasmas. We also work on the improvement of simulation, both theoretically and practically.

Our staff is:

Professor C. K. Birdsall *Principal Investigator*	191M	Cory Hall	(643-6631)
Dr. Kim Theilhaber *Post-doctorate*	187M	Cory Hall	(642-3477)
Mr. William Lawson	199MD	Cory Hall	(642-1297)
Mr. Niels Otani	199MD	Cory Hall	(642-1297)
Mr. Richard Procassini	199MD	Cory Hall	(642-1297)
Ms. Lou Ann Schwager *Research Assistants (students)*	199MD	Cory Hall	(642-1297)
Perry Gray *Senior Engineering Aide*	199MD	Cory Hall	(642-1297)

Our Advisors and Associates are:

Dr. Ilan Roth *Physicist, Space Science Lab., UCB*	304	SSL, Campus	(642-1327)
Dr. Bruce Cohen	L630	LLNL, Livermore	(422-9823)
Dr. Alex Friedman	L630	LLNL	(422-0827)
Dr. A. Bruce Langdon	L472	LLNL	(422-5444)
Dr. William Nevins *Physicists, Lawrence Livermore Natl. Lab.*	L630	LLNL	(422-7032)

June 30, 1986

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ELECTRONICS RESEARCH LABORATORY

University of California
Berkeley, California 94720

This report was produced by Carole Frank

Table of Contents

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SECTION I: GENERAL PLASMA THEORY AND SIMULATION

A. Computer Simulation of Bounded Plasma Systems

William S. Lawson

Abstract

The physical and numerical problems of kinetic simulation of a bounded electrostatic plasma system in one planar dimension are examined, and solutions to them are presented. These problems include particle absorption, reflection and emission at boundaries, the solution of Poisson's equation under non-periodic boundary conditions, and the treatment of an external circuit connecting the boundaries. Some comments are also made regarding the problems of higher dimensions. The methods which are described here are implemented in a code named PDW1, which is available from Professor C. K. Birdsall, Plasma Theory and Simulation Group, Cory Hall, University of California, Berkeley, CA 94720.

This work is to be issued as Memorandum No. UCB/ERL M87/14, March 5, 1987.

B. Artificial Cooling of Trapped Electrons in Bounded Simulations

William S. Lawson

Abstract

An explanation is proposed for an artificial cooling effect seen in electrostatic particle-in-cell plasma simulations. Further simulations are done which test and support the explanation.

A report with the title shown above is in preparation, Memorandum No. UCB/ERL M87/34, as well as for journal submission. The final title may be altered slightly.

Projects reported as A,B,C,D,E,F in the previous QPR (III & IV, 1985) have been completed and final reports have been issued.

SECTION II: PLASMA-WALL PHYSICS, THEORY AND SIMULATION

A. **Collector Sheath, Presheath, and Source Sheath in a Collisionless, Finite Ion Temperature Plasma**

Lou Ann Schwager

B. **Potential Drop and Transport in a Bounded Plasma with Ion Reflection at the Collector**

Lou Ann Schwager

C. **Potential Drop and Transport in a Bounded Plasma with Secondary Electron Emission at the Collector**

Lou Ann Schwager

Final reports with the above titles are in preparation for ERL memos and journal submissions. The final titles may be altered slightly.

D. **Magnetized Sheath; Kelvin-Helmholtz Instability; Long-lived Vortices**

Dr. Kim Theilhaber

In performing two-dimensional simulations of a magnetized sheath, we expect to reveal important physical behavior which is not described by the one-dimensional simulations, in particular time-varying electric field fluctuations sustained by plasma instabilities, and intrinsically two-dimensional particle transport across the discharge. We have been using our two-dimensional particle simulation code ES2 to model a bounded plasma in a plane perpendicular to the magnetic field, along the midsection shown in Fig. 1, page 8, QPR III & IV, 1985. In this configuration, the walls of the device lie parallel to the y direction, and are separated by a distance in the x direction, with the magnetic field parallel to z. Because the electric fields in the plasma are spatially non-uniform, and give rise to a highly sheared **E** x **B** drift of electrons and ions in the y-direction, the discharge will be unstable to the so-called "Kelvin-Helmholtz" instability, an instability which feeds on the free energy contained in the sheared flow. In the long term, starting from an initially laminar flow, the Kelvin-Helmholtz instability drives the particle motion into a set of vortices, through which some but not all of the free energy in the shear layer is dissipated.

A snapshot from an ES2 simulation, in which the Kelvin-Helmholtz instability was present, is shown in Fig. 1. This figure shows the electrostatic potential contour lines for the final, quasi-steady state of the instability, at $\omega_{ci}t \approx 100$, in a system which was initially filled with a uniform plasma. This particular situation did not faithfully reproduce the conditions of the magnetized sheath, in particular because there was no external bias imposed across the system; rather, it was meant as a preliminary exploration of the model. In the simulation, the wall potentials were left floating, and the initial shear flow was provided by the electric field generated by charge deposition at the walls, due to the depletion, over a layer of the order of an ion gyro radius in width, of ions near the wall. The system pictured in Fig. 1 is about 5 ion gyro radii across, and about 20 ion gyro radii long in the direction parallel to the walls. While the initial vortices, which develop out of the Kelvin-Helmholtz instability at $\omega_{ci}t \approx 20$ are localized near the walls, in Fig. 1 we are looking at the potential at the later time $\omega_{ci}t \approx 100$, and the vortices have expanded in x so as to occupy the entire system. The potential perturbations induced by the vortices are sizeable, $e\phi / T_i \approx 0.5$. They carry along comparable perturbations in the particle density, with $\delta n / n_o \approx 0.5$.

The most striking feature of the vortices is their great stability: the vortices on the left move with a steady motion parallel to the wall, in accordance with the **E x B** drift, while those near the right wall stream in the opposite direction with equal speed. The vortices overlap and pass through each other with little effect on their shapes and amplitudes.

An important consequence of the presence of vortex motion in the plasma is the rate of particle transport to the walls, which is enhanced over the collisional rate. In the simulation of Fig. 1, the enhanced transport resulted in the depletion of almost all particles in the simulation region, over a time scale much shorter than the collisional time scale. We are presently studying the dependence of this "anomalous" transport on the vortex structure and on the plasma parameters. Another important feature of the vortices, which should be observable in an experiment, is that they produce a high-frequency power spectrum, which peaks at $\omega \approx k_y v_D$, where v_D is the characteristic drift velocity, and k_y the characteristic wave vector of the potential fluctuations parallel to the wall.

We expect behavior similar to that discussed above in a fuller model of the magnetized sheath, with nonzero bias. The enhanced transport due to the vortices should be especially important in the magnetized sheath, as we believe that this might modify the sputtering efficiency of the device. Two-dimensional particle simulations are now under way to study how this efficiency might be affected, and how it depends on the plasma parameters such as density and magnetic field.

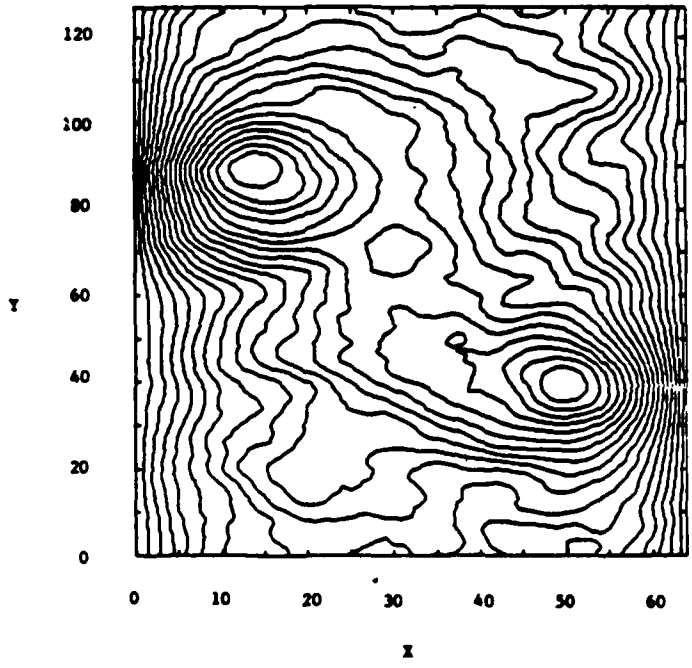


Fig. (1): Contour plot of the electrostatic potential $\varphi(x,y)$, at $\omega_{pi}t = 100$, in a bounded plasma simulation, using the code "ES2". The confining walls are at x=0 and x=64, the external magnetic field is perpendicular to the plane of the simulation region. The left-hand vortex is streaming down the wall with a velocity of about 0.1 v_{ti}.

SECTION III: CODE DEVELOPMENT AND SOFTWARE DISTRIBUTION

A. ES2 User's Manual--Version 1

Dr. Kim Theilhaber

Abstract

The two-dimensional, electrostatic plasma simulation code "ES2" is described. This includes a synopsis of the physical basis of the model and a summary of the numerical schemes used to implement it. This is followed by two examples of applications, one showing the formation of unmagnetized double layers, the other illustrating the formation of vortices in a configuration perpendicular to the magnetic field. Finally, the main section of the manual is presented: a copy of the "on-line" manual, in which a detailed description of the various options and parameters entering into ES2 is given.

This work has been issued as an ERL Memo No. UCB/ERL M87/23, May 11, 1987.

B. Addition of Electron-Neutral Elastic Collisions

Perry Gray (write-up by Prof. C. K. Birdsall)

Electron-neutral collisions may be accounted for in simulations, as for application to low-pressure discharges. Let the electrons collide with hard sphere neutral atoms, so that the collisions are elastic (no momentum transfer) and the electrons are scattered randomly with a uniform distribution in velocity angle, independent of their initial velocity angle.

The details of this program and the checks performed will be given in a later QPR.

C. Implicit Particle Simulation of Velocity Space Transport and Self-Consistent Electric Potentials in Magnetized Plasmas

TESS Code

R. J. Procassini, C. K. Birdsall and E. C. Morse
and
B. I. Cohen (Lawrence Livermore National Laboratory)

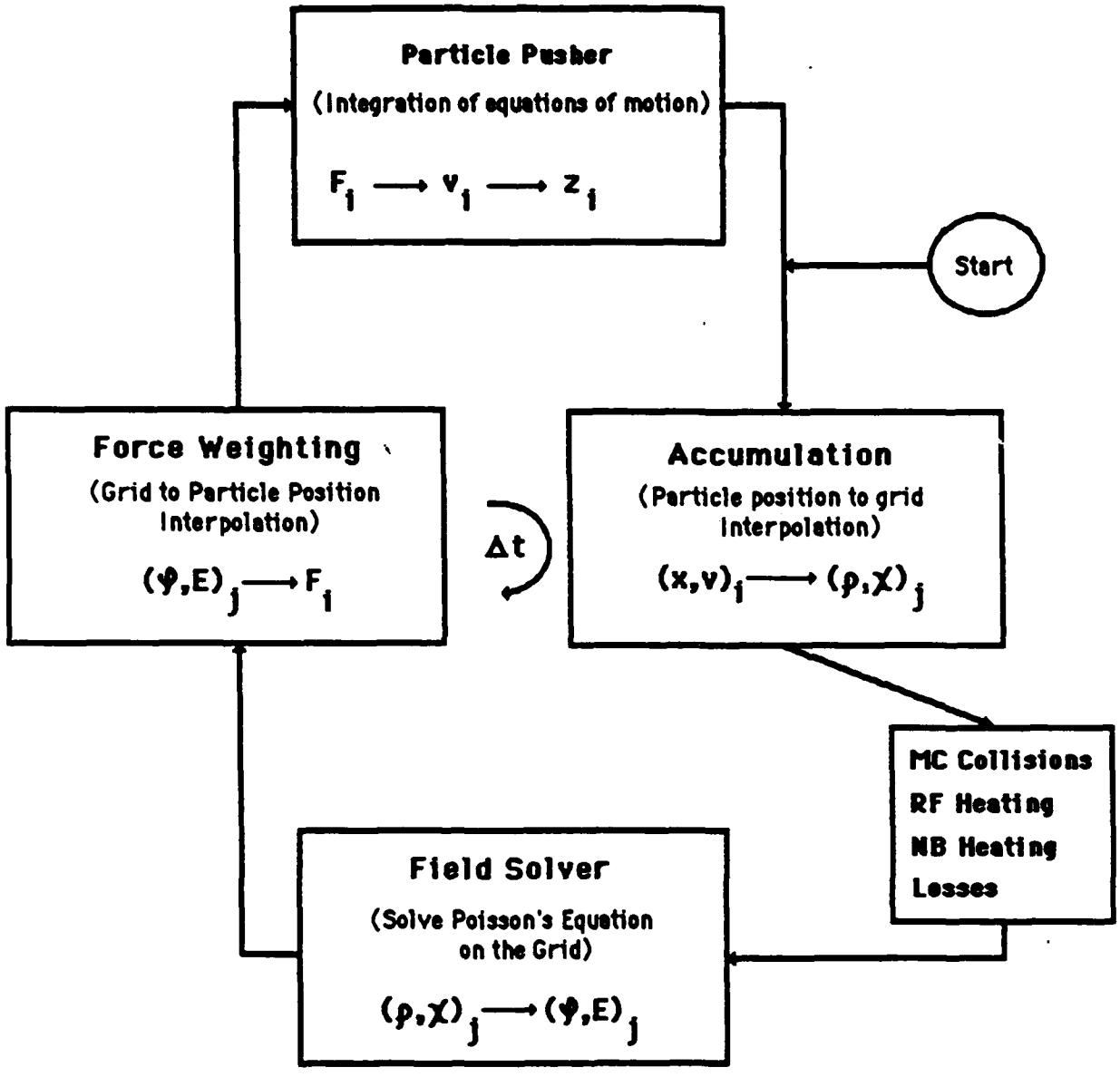
Introduction

We are developing a one-spatial-dimension, three-velocity-component implicit particle simulation code incorporating binary particle Coulomb collisions self-consistently to simulate velocity space transport and electric potentials in magnetized plasmas. The simulation model addresses long transport time scales, which are not accessible to explicit algorithms, and retains essential kinetic details. This new simulation tool is an efficient alternative to Fokker-Planck codes. The implicit potential solver, particle pusher, and collision routines have been successfully implemented and tested. Rudimentary simulations of a Q-machine and a simple tandem mirror configuration have been performed. In the near future, we will add physics packages to model radiofrequency wave heating, plasma fueling by gas-puffing , neutral beam heating and fueling, and particle losses. At that point, we will be able to simulate thermal barrier tandem mirror operation. Figure 1 shows a schematic representation of the timestep cycle of the code, including the particle pusher, field solver, and collision, heating and particle loss routines.

Objectives

We are combining recently introduced implicit particle simulation methods[1] with Monte Carlo model of binary particle collisions, neutral beam ionization and

Schematic Description of the Computational Sequence--



(i ≡ Particle Index ; j ≡ Grid Point Index)

Figure 1. The TESS Computational Sequence.

charge exchange. and radiofrequency wave heating to perform simulations of both velocity-space transport and the evolution of the self-consistent plasma electric potential. We intend to demonstrate that this new simulation tool is a very flexible and efficient alternative to the Fokker-Planck codes that are very widely used in the plasma physics community. Our simulation model is particularly well suited to many magnetic fusion configurations (tandem mirrors, theta pinches, Q-machines, tokamak divertors) and magnetospheric double-layer phenomena. Our first applications will be to the study of electrostatic particle confinement and the formation of electrostatic thermal barriers in tandem mirrors. Figure 2 shows the particle and energy sources and sinks in one-half of a symmetric tandem mirror experiment. This is the calculational domain of our axial, one-spatial-dimension model.

Progress

Significant progress has been made in development and testing of the **TESS** (**T**andem **E**xperiment **S**imulation **S**tudies) code in the areas of code/algorithm optimization and rudimentary physics applications.[2] A study was completed in which the performance of two alternative implicit differencing schemes was compared to determine which scheme minimized numerical heating and cooling. This study was based upon the free expansion of an overall charge-neutral plasma slab. We investigated operating regimes for the two algorithms with respect to the important parameters $\omega_{pe}\Delta t$ and $\Delta x/\lambda_{De}$, where ω_{pe} is the electron plasma frequency, Δt is the time step, Δx is the grid spacing and λ_{De} is the electron Debye length. An optimum value of $\Delta x/\lambda_{De} \approx 3\omega_{pe}\Delta t$ for $\omega_{pe}\Delta t > 1$ was determined. Values of $\omega_{pe}\Delta t$ as large as 50 were successfully tested, and larger values can be accommodated.

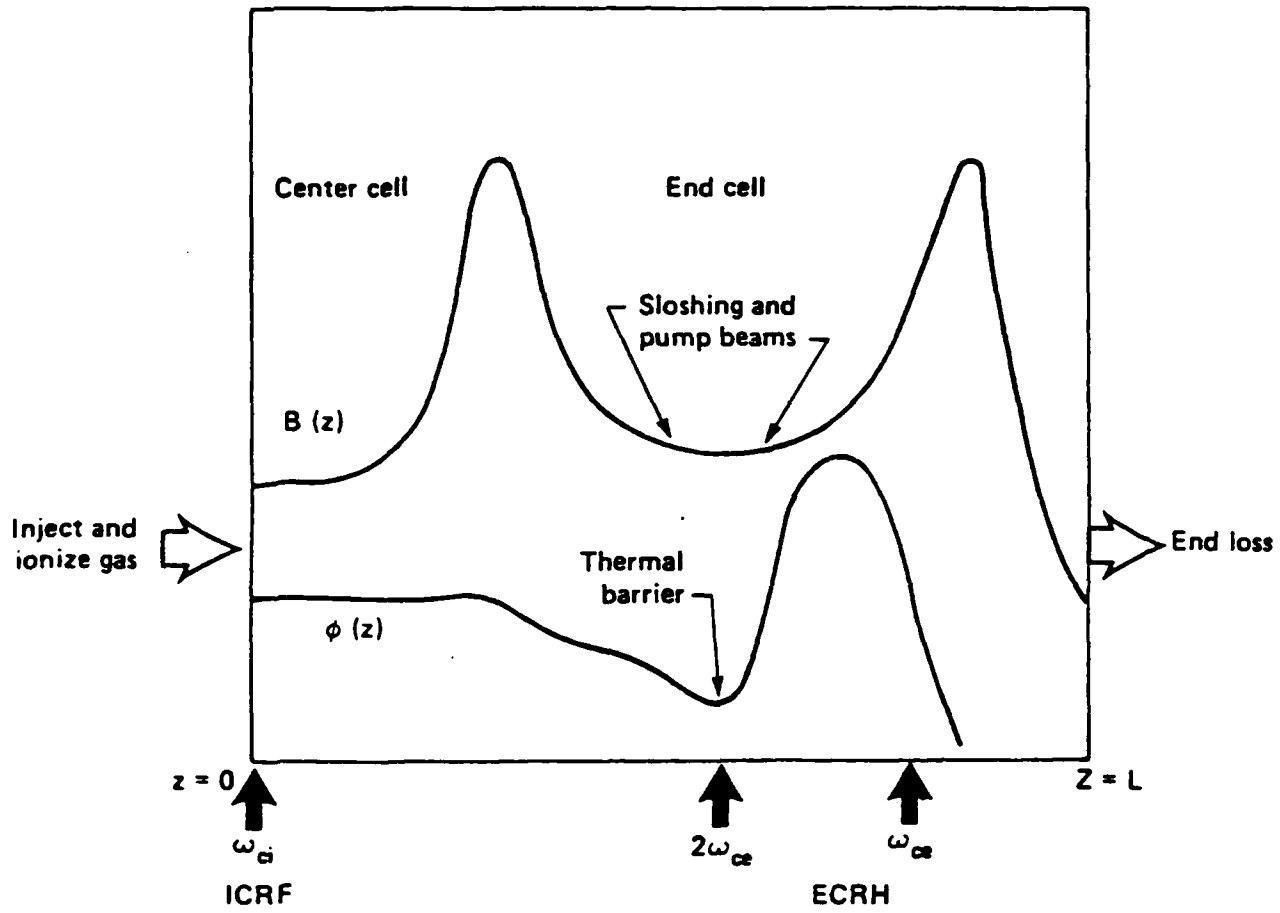


Figure 2. Schematic drawing of the 1-D axial model of thermal barrier formation in a tandem mirror, indicating the principal sources of particles and heating.

We also completed and successfully tested a subroutine for binary particle Coulomb collisons. This major physics package models screened Coulomb collisions self-consistently, i. e. the distribution function evolves due to the collisions, both momentum and energy are conserved, and the entropy of the plasma either increases or remains constant. Furthermore, the collision kinematics are relativistic, and the Monte Carlo scattering is algorithm is vectorized. A complete set of textbook examples of collisional relaxation processes have been simulated and reported. Detailed descriptions of the implicit differencing scheme performance study and the becnchmarking of the binary particle collision routine will be presented in future Quarterly Progress Reports.

Our first physics applications including self-consistent electric potentials have been the simulation of a plasma in contact with an insulated conducting wall. The observed potential drop to the wall and its dependence on electron and ion temperatures agree with analytical sheath models. We have made similar simulations including the influence of applied magnetic mirror fields on the plasma confinement. These studies have provided a very valuable testbed: they quantitatively establish the sensitivity of the simulation results to numerical discretization and statistical noise, and clearly demonstrate that **TESS** successfully combines particle simulation, Monte Carlo and Fokker-Planck simulation tools.

Future Development

The implementation and testing of the remaining physics packages (wave heating, neutral beam ionization and charge exchanges, axial and radial particle losses) over the next several months will enable us to perform realistic thermal barrier

tandem mirror simulations. thereby establishing credibility in the physics value of **TESS**. We will then compare **TESS** to existing Monte Carlo and Fokker-Planck codes. We will also continue our study of simulation performance characteristics and explore possibilities for multi-stepping (sub-cycling) and orbit averaging of the particle data to improve the efficiency of the code.[3] Longer term goals include the extension of **TESS** to two spatial dimensions and different magnetic field geometries.

References

[1] A. Friedman, A. B. Langdon and B. I. Cohen, "A Direct Method for Implicit Particle-In-Cell Simulation", *Comments Plasma Phys. Contr. Fusion*, **6**, 225(1981).

[2] R. J. Procassini, C. K. Birdsall and B. I. Cohen, "Direct Implicit Particle Simulation of Tandem Mirrors". *Bull. Amer. Phys. Soc.*, **31**. 1621(1986).

[3] B. I. Cohen, "Orbit Averaging and Subcycling in Particle Simulation of Plasmas", in **Multiple Time Scales**(eds. J. U. Brackbill and B. I. Cohen), *Computational Techniques*, Academic Press, London(1985).

D. Dynamic Dimensioning with Heap Management

Lou Ann Schwager

I. Introduction

Dynamic dimensioning is useful for those who need to automatically increase array lengths in a computer program during run time. In particular we present this guide to demonstrate the use of dynamic dimensioning in particle simulation codes. This technique allows for adding memory to arrays just before their pre-set array length is exceeded during a run. We highly recommend that the interested user acquire a copy of the memory management section in the BASELIB document before attempting any of this. (Use DOCUMENT VIEW BASELIB with keyword "heap-management" and keywords for individual routines.)

For particle simulation codes, certain arrays, such as position and velocity for each particle, have a length dependent on the maximum number of particles *npmax*. Usually the user specifies *npmax* in the code prior to compilation which sets the lengths of the arrays. If that value is too small, then the run terminates (or generates an error downstream) when array lengths are exceeded. Then the entire computation costs are wasted. Also for a simulation model that generates new particles with time and starts void of particles then, through most of the run, much unused space exists in the particle dependent arrays. Those users familiar with the NMFECC system realize that a larger program field length requires either a higher priority (and thus a higher cost charged for computation) or more personal time invested. To mitigate these two problems, using dynamic dimensioning can avoid the case of premature termination and can reduce the average cost of a run. Especially improved are those runs requiring over 10,000 total particles and over ten minutes of Cray-1 computation time. Memory management does cost some i/o and system time so that optimally it should be called on only a few times during a run.

II. Technique Implementation

Usually array lengths are specified in the code prior to compilation. Hence to use memory management, before compilation we set the length of these expandable arrays to one. In the coding before any of these arrays are referenced, the initial values for these lengths are read in from the

input file. Then we call on the heap manager to allocate a moveable block of memory for each expandable array.

Before embarking on how to accomplish the initial allocation, we must explain the use of pointers in memory management. (Pointers are discussed in the CFT document under keyword "pointer-statement".) Pointers, which have integer type, provide the base address of an array or variable. Changing the value of a pointer moves the location of the entire array. The pointer statement for a particular array must reside in the routine of use. This restriction exists because the pointered array cannot be passed into a routine as a dummy argument or in a common block; whereas the pointer itself can be.

Pointers can be passed through labeled common blocks to the subroutine where memory is managed. Using the BASELIB routine MZMALLOC for each array assigns the initial moveable block of memory. The first argument of MZMALLOC is the pointer of the array and the second argument is the block length in words. The array can also be dimensioned in the pointer statement. Note that error status is returned when almost any of the MZ routines are called. When the error status equals zero, the task has completed successfully. Hence nonzero values should be trapped and the run suspended or terminated. (See the BASELIB document for details.) At this point in implementing the above changes, the user can test the program by choosing a value of *npmax*, in the input file, which will not be exceeded during a run.

As the run proceeds and array values are assigned, a test assesses whether the array length is about to be exceeded. When this occurs, that routine should call the subroutine which lengthens the array blocks. (Placing this expansion routine in a separate subroutine, though not required, facilitates debugging.) The BASELIB routine MZCHANGE expands an allocated block of memory. Its first argument is the pointer for the array and the second is the total new block length. The BASELIB routine MZSTATUS can be called on to provide, for curiosity's sake, the free space available after each MZCHANGE call. The BASELIB routine IZPROGFL provides the program field length.

In printing all the pointer values, program field length, and available free space, the curious user can observe how the heap manager shuffles the newly expanded arrays. Usually with the first call to the expansion subroutine, the first array changed is moved to an address larger than that of the last array. ("Last" is defined as the final array initially allocated memory with MZMALLOC.) The second array changed may move beyond the first array or may move into the old space of the first array. This shuffling depends on the amount of extra length added and the array size. Obviously after several calls to the expansion subroutine, the relative base addresses of these arrays are considerably scrambled from the original positions. Consequently if the user employs a pointer which depends on the value of an array's base address, then this pointer must be updated after all changes. The heap manager only returns the new value of the array's base address.

We observe that, with only using MZCHANGE, after the heap manager juggles all the arrays in the expansion routine, a considerable amount of free (unallocated) space exists. The BASELIB routines MZPARAM and MZPACKH are used to reduce this free space. Thus the minimum program field length is maintained during the run until the expansion routine may again be called. Deciding how and when to use these two routines requires some operating experience.

The user sets the second argument, *epsilon*, and the fourth argument, *maxfat*, in the array required as input for an MZPARAM call. This *epsilon* value sets the amount of extra space allowed to accompany a changing block. Consultants recommend that it be set to no less than the shortest block length. The value *maxfat* specifies the maximum space allowed to accumulate at the end of the heap before the heap manager removes the excess and shortens the program field length. The default for *maxfat* is 32. Because the heap manager can shorten the field length without provocation, we fix *maxfat* initially to a large value such as the largest block size. Then after all arrays are expanded (at the end of the expansion routine) we set *maxfat* back to 32 and then call MZPACKH.

Next calling MZPACKH repacks the heap to move free space, according to *epsilon*, to the end of the heap. Then the heap manager automatically removes the extra end space (beyond *maxfat*). The argument for MZPACKH is set equal to zero. As it currently stands, MZPACKH will shuffle a

block of memory (to consolidate free space) only if sufficient, contiguous free space exists to shuffle the allocated block into. In other words, MZPACKH is not smart enough (as yet) to slide blocks around the small extra spaces, even if *epsilon* were set less than the smallest block length.

With dynamic dimensioning, we provide the caveat that, although array space may be allocated, strange errors ensue if an array element is referenced before its value is initialized. Because the garbage residing at the referenced, uninitalised location may propagate through the code, an overflow/underflow error may appear several subroutines later.

III. Technique Demonstration

The particle simulation code **PDW1** is used to illustrate the dynamic dimensioning technique. In **PDW1** the position and velocity arrays are assigned pointers in the routine MAIN. Other particle-dependent arrays, such as flags for certain locations within the simulation system, are pointered in the subroutine where these flags are set. For example, in MAIN the pointer statement for position array x is $pointer(px, x(1))$. The pointer px passes through a common block to subroutine START where the heap manager allocates memory via $ierr = mzmalloc(px, npmax * nsp)$ where nsp is the number of species. Memory for all the expandable arrays is allocated initially in subroutine START. In **PDW1** the test for exceeding the maximum number of particles $npmax$ occurs while particles are added during a call to LOAD or ADJUST. If the test is true, then subroutine EXPAND is called.

Suppose that the particle-dependent arrays are position x, velocity v, and some flag if. The x and v arrays have length $npmax * nsp$ and if has length $npmax$. The x and v arrays contain the values for species stacked in one-dimension (rather than in nsp-dimensions). Consequently the elements in array $nloc$, which mark the beginning of each species, must also be increased with the new $npmax$ after EXPAND is called. The expansion routine EXPAND follows.

```
      subroutine expand(npmax,nsp,nloc)
      use maxpar
c*    Below are the three pointers which locate the base address
c*     of each respective array: x, v, and if
      common /pmain/ px, pv
      common /pflag/ pif
      common /shuffle/ nadd
      dimension nloc(nsmax1), kparam(4)
      data kparam(1)/-1/, kparam(3)/-1/, kpackh/0/
      integer px, pv, pif
c*    Nadd, the memory added, is the user's best guess which
c*     affects the number of times EXPAND may be called
      nadd = 5000
c*    Update npmax and nloc
      npmax = npmax + nadd
      do 10 i=1,nsp
      nloc(i+1) = i * npmax
 10   continue
c*    Set maxfat and epsilon
      kparam(2) = npmax
      kparam(4) = npmax * nsp
      iparam = msparam(kparam,4)
c*    Expand each array and print status.
c*    The error value ichange is incremented by ten with
c*     each mxchange to aid in locating errors and in
c*     understanding the status printout.
c*    With a correctly completed task, the mxchange value is zero.
      ichange = mschange(px,npmax*nsp) + 10
      if(ichange.gt.10) goto 20
      call status(ichange)
      ichange = mschange(pv,npmax*nsp) + 20
      if(ichange.gt.20) goto 20
      call status(ichange)
      ichange = mschange(pif,npmax*nsp) + 30
```

```
      if(ichange.gt.30) goto 20
c*    Reset maxfat to default and repack heap
      kparam(4) = 32
      iparam = mzparam(kparam,4)
      ipackh = mzpackh(kpackh)
      call status(ichange)
      go to 30
 20   call finish
 30   continue
      return
      end
      subroutine status(ichange)
c*    Print program length, free space, and pointer values
c*     in OUTPUT.
      common /pmain/ px, pv
      common /pflag/ pif
      dimension aprog(3), kstat(2)
      iprog = isprogfl(aprog)
      istat = mzstat(kstat,2)
      write(3,11) kstat(2),aprog(2),px,pv,pif,ichange
 11   format(1x,"STATUS: free space=",i6,"field length=",i8,/,
     *   "px=",i8,"pv=",i8,"pif=",i8,"for ichange=",i3)
      return
      end
```

With x and v newly expanded, if the program adds a particle of the first species, then the first element in x and v for the second species will be overwritten. Consequently we must distribute the extra space allocated, which is now residing at the end of each array, internally to the end of each species. Immediately after calling EXPAND, we then call the subroutine SHUFFLE which follows below.

```
      subroutine shuffle(s,nloc,nsp)
c*    Redistribute memory for species-dependent array s
      common /shuffle/ nadd
      dimension s(1), nloc(1)
c*    Routine MOVE (in FORTLIB) moves array sections to
c*     new addresses within that array.
c*    Note that in PDW1 the suboutine MOVE must be renamed.
      imove = nloc(2) - nadd
      do 10 isp=nsp,2,-1
      moveto = nloc(isp) + 1
      movefrm = nloc(isp) - (nadd*(isp-1)) + 1
      call move(s(moveto),s(movefrm),imove)
 10   continue
      return
      end
```

For any species-dependent array, subroutine SHUFFLE must be called just prior to its next reference during the run. For example, if such an array is in subroutine OUTPUT, then it is not referenced right after the call to EXPAND (in ADJUST or LOAD) but perhaps many time steps later. Hence we can set a flag in EXPAND which is passed via a named common block to OUTPUT. When this flag is true then we call SHUFFLE (from OUTPUT) and then reset the flag to false.

IV. Conclusions

Hopefully the above discussion covers most of what the user may need to undertake the use of dynamic dimensioning. This technique can also be used, for example in matrix inversion, to allocate and deallocate memory should a large array be temporarily required. The whole process also educates the user, who previously was familiar only with the old linkage (link=0) system, on the strange new creature of the link=2 system called the heap and its management.

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SECTION IV: JOURNAL ARTICLES, REPORTS, TALKS, VISITS

Journal Articles

Charles K. Birdsall, Niels F. Otani and Bruce I. Cohen, "Simulation of Plasma Dynamics Using Many Particles," *IEEE Electrotechnology Review* 2, pp. 43,44, 1986.

Reports

Niels F. Otani, "Saturation and Post-Saturation Behavior of the Alfvén Ion-Cyclotron Instability: A Simulation Study," University of California, Berkeley, Memorandum No. UCB/ERL M86/15, 19 February 1986.

Niels F. Otani, "Stabilizing Effects of Finite-Amplitude RF Waves on the Interchange Instability," University of California, Berkeley, Memorandum No. UCB/ERL M86/18, 28 February 1986.

William S. Lawson, "Limits of Linear Response of a Vlasov Distribution," University of California, Berkeley, Memorandum No. UCB/ERL M86/44, 3 June 1986.

Charles K. Birdsall, Niels F. Otani and Bruce I. Cohen, "Simulation of Plasma Dynamics Using Many Particles," University of California, Berkeley, Memorandum No. UCB/ERL M86/47, 3 June 1986.

K. Theilhaber, G. Laval and D. Pesme, "Numerical Simulations of Turbulent Trapping in the Weak Beam-Plasma Instability," University of California, Berkeley, Memorandum No. UCB/ERL M86/50, 5 June 1986.

Poster Paper at Sherwood Theory Conference, New York, N.Y., April 14-16, 1986, abstract in QPR III, IV, 1985.

Niels F. Otani and Bruce I. Cohen, "Effect of Large-Amplitude Perpendicularly-Propagating RF Waves on the Interchange Instability"

Minicourse

Prof. C. K. Birdsall presented the topic "Plasma Simulation using Many Particles" at the *IEEE Minicourse on Generation of High-Power Microwaves, Millimeter- Waves, and Submillimeter Waves*, Saskatoon, Canada, 21-23, 1986. His presentation will be published as a chapter in a book edited by Profs. Igor Alexeff and Victor Granatstein.

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